

Industrial Needs for Powder and Single Crystal Diffraction

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INEOS
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Industrial problem solving
is almost by definition
multi-hamlet and multi-village!

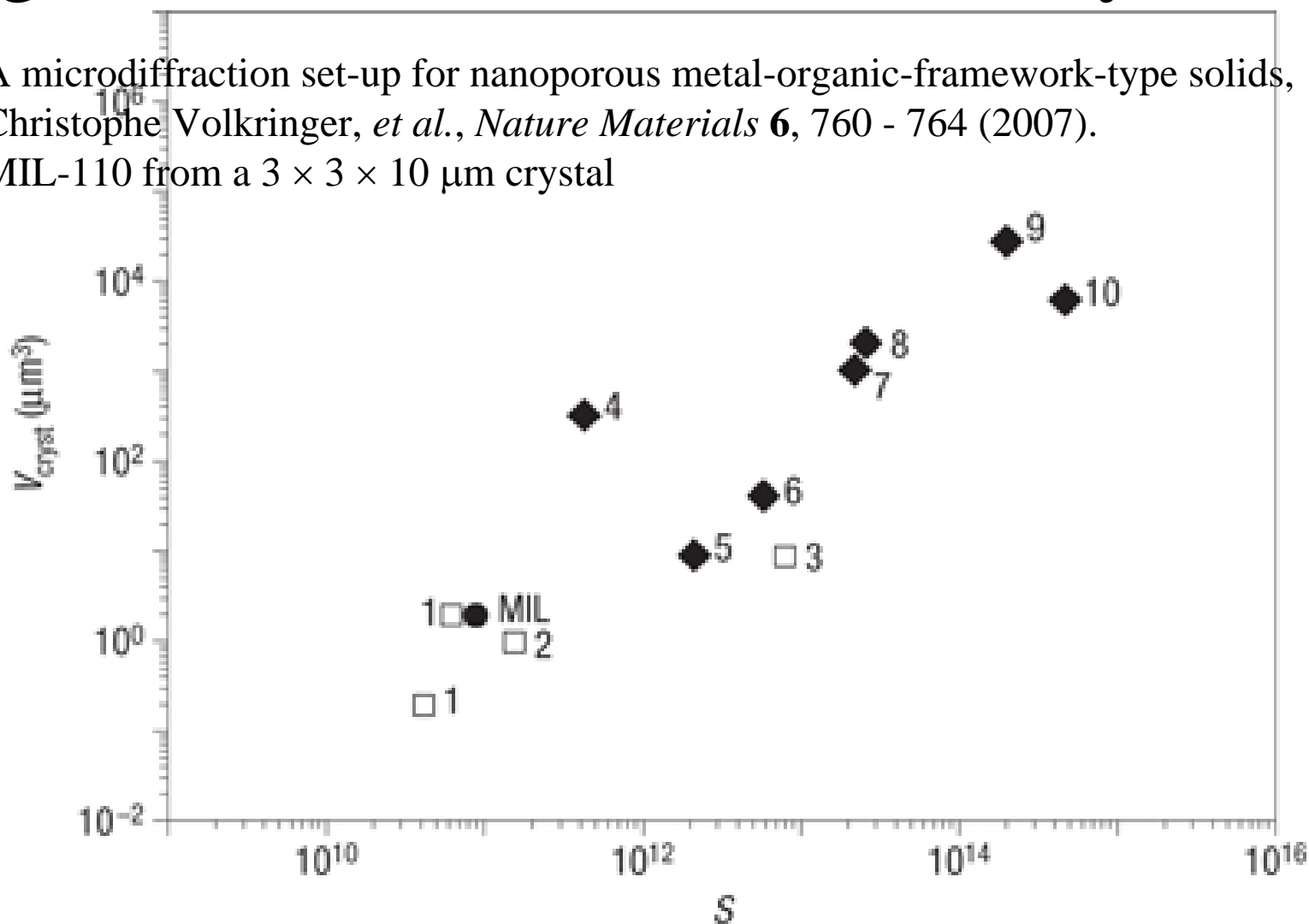
The synchrotron is an extension
of the home lab.

Single Crystal Diffraction

get the model (from a microcrystal)

A microdiffraction set-up for nanoporous metal-organic-framework-type solids,
Christophe Volkringer, *et al.*, *Nature Materials* **6**, 760 - 764 (2007).

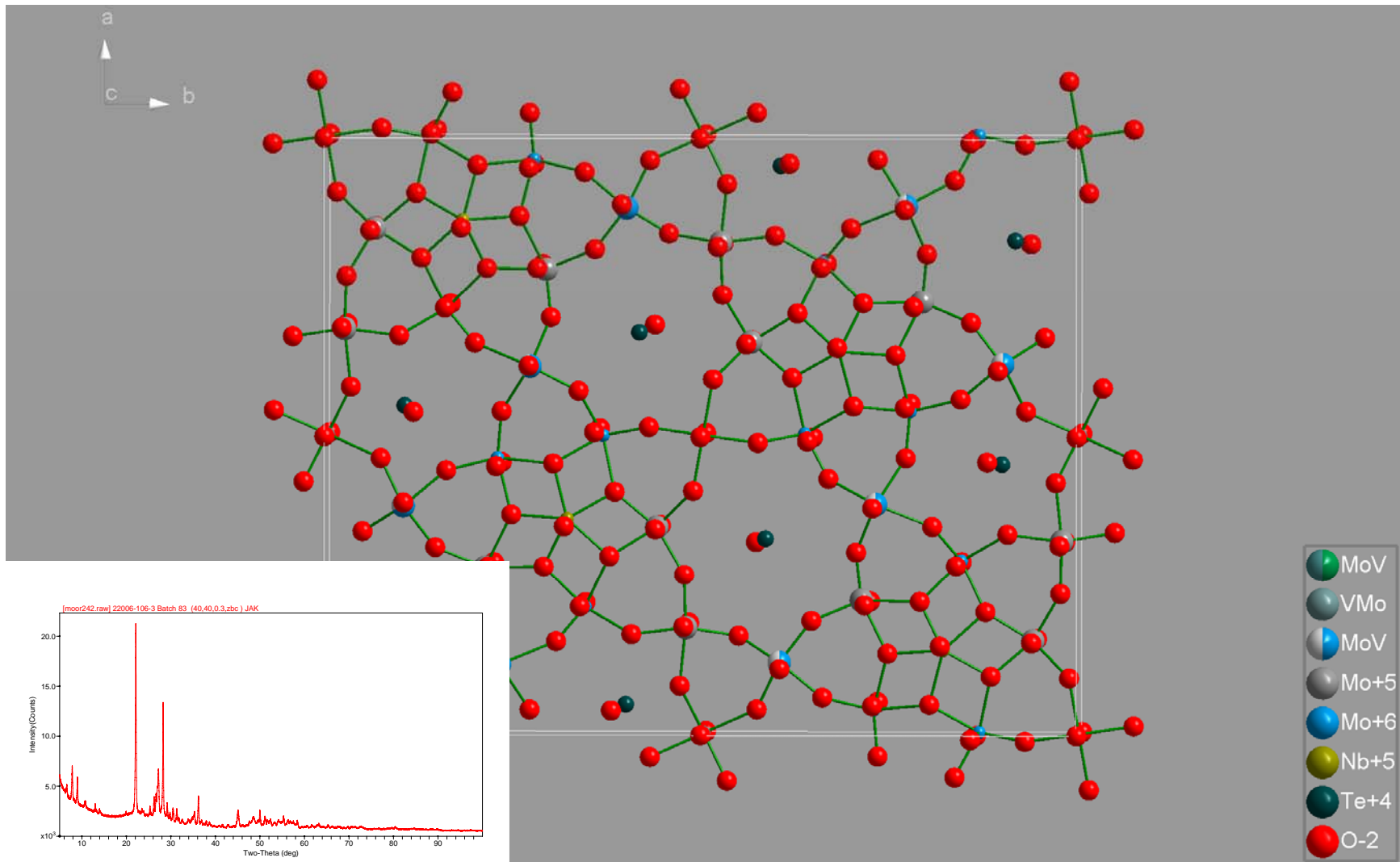
MIL-110 from a $3 \times 3 \times 10 \mu\text{m}$ crystal



Powder Diffraction

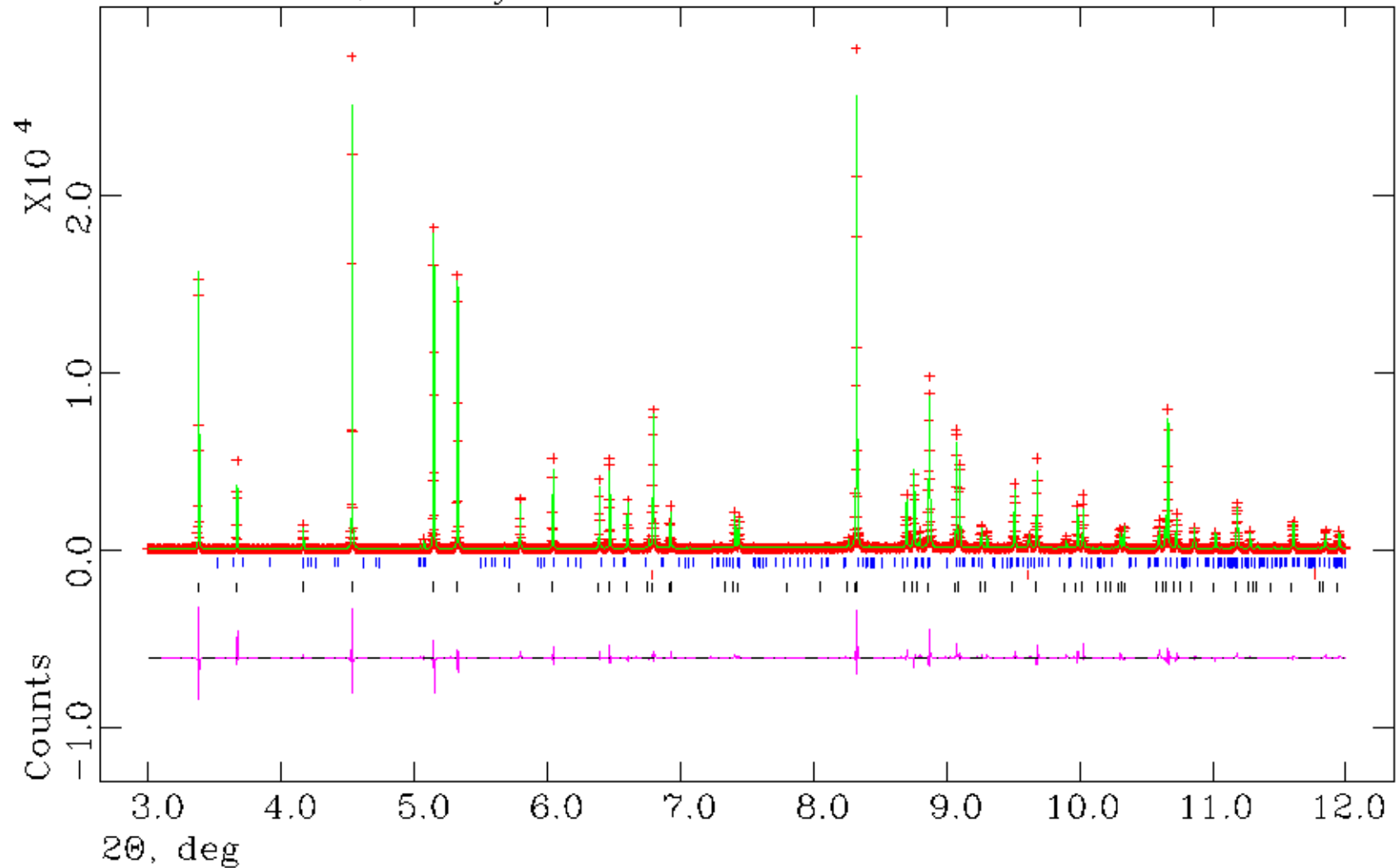
- Structure solution and refinement
- Micro(nano)structure characterization
- *In situ* characterization of real systems

Multiple Partially-Occupied Sites



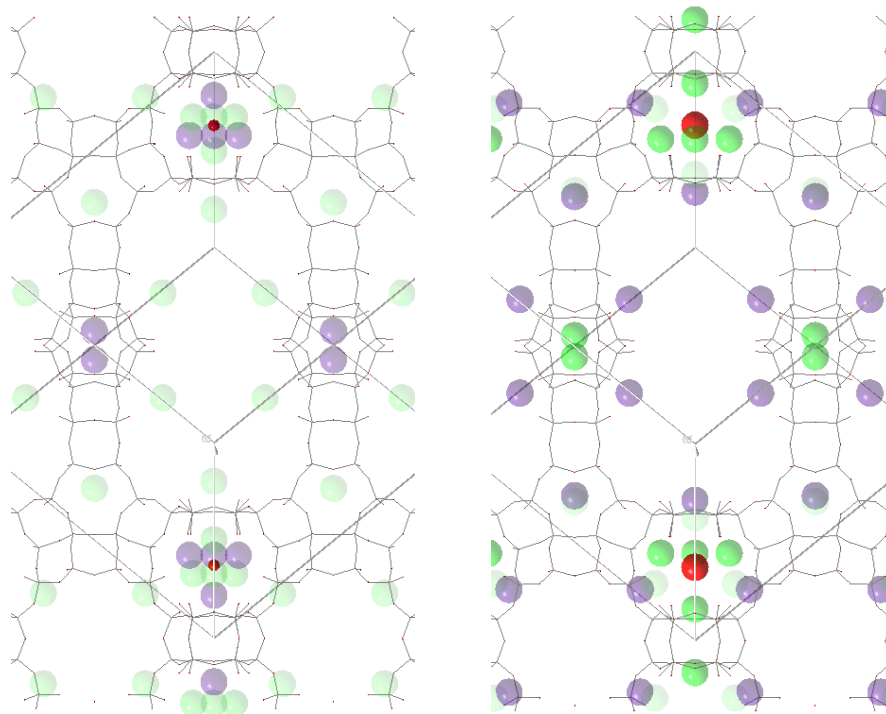
Profile Shapes

21031-38-1, (N H₄)₃ (Zn Cl₄) Cl, ID10 1 mm capillary (NZN Hist 1
Lambda 0.4591 Å, L-S cycle 320 Obsd. and Diff. Profiles



In situ Characterization

Every catalyst I have ever characterized at reaction conditions has had a different structure than at ambient conditions!



RT

300°C

Environments

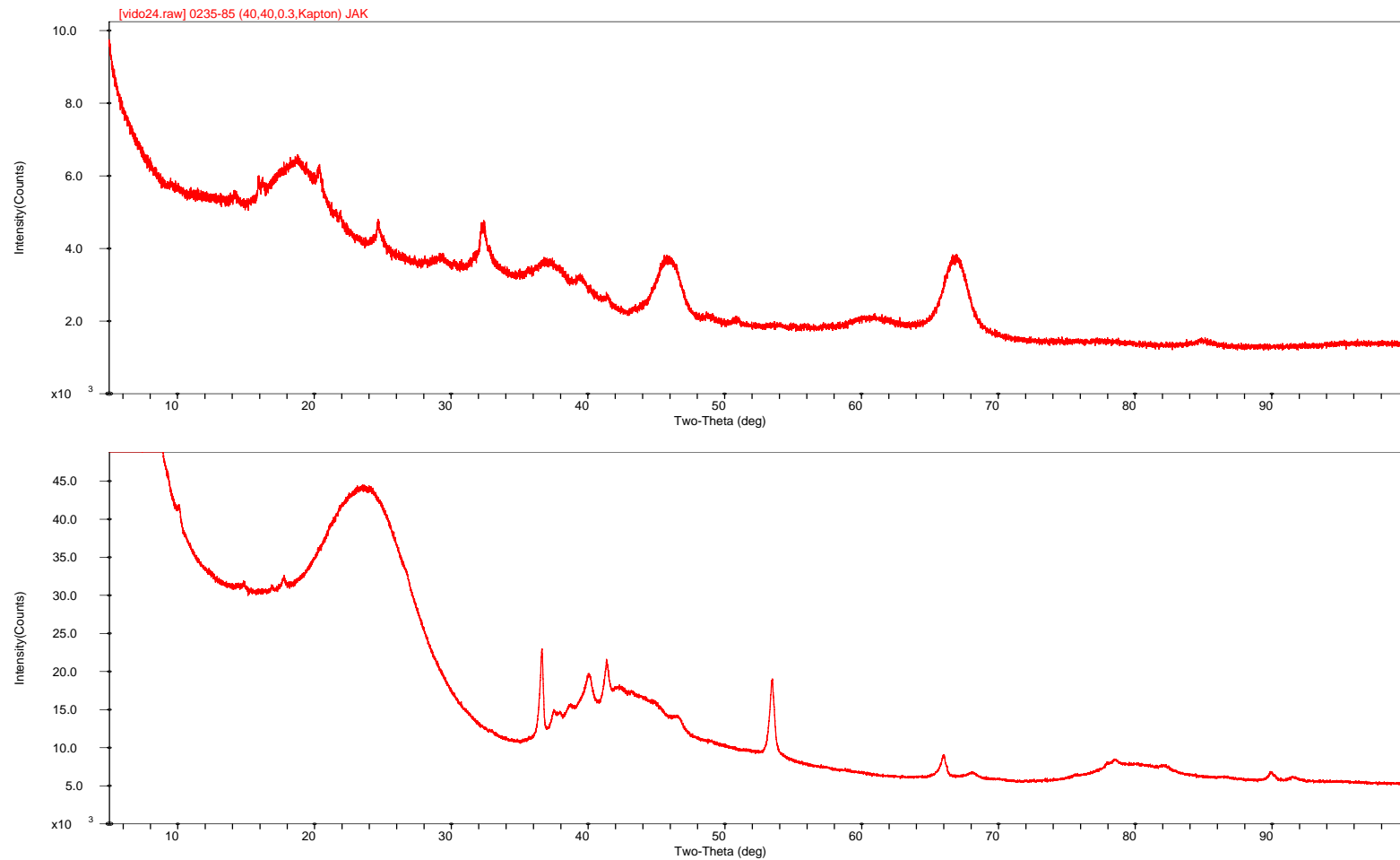
- Vacuum, nitrogen, helium
- 3000 psig hydrogen
- Butane + air
- Propylene + air + ammonia
- ...

Put the beam *there*

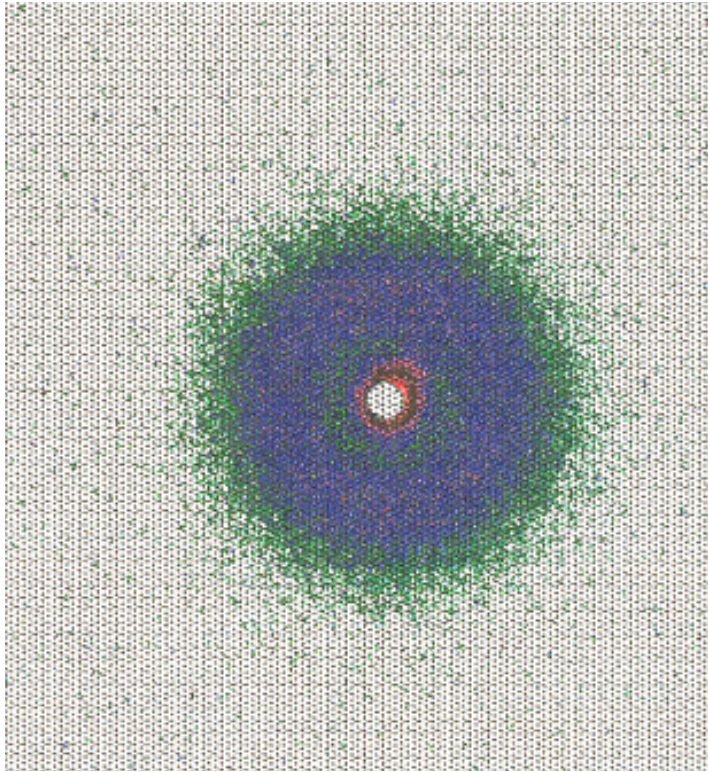
- Interactions between phases (interfaces) in a polycrystalline catalyst
- A particular spot in a catalyst particle
- Defects, inclusions, impurities, failures

(environmental SEM at sample position?)

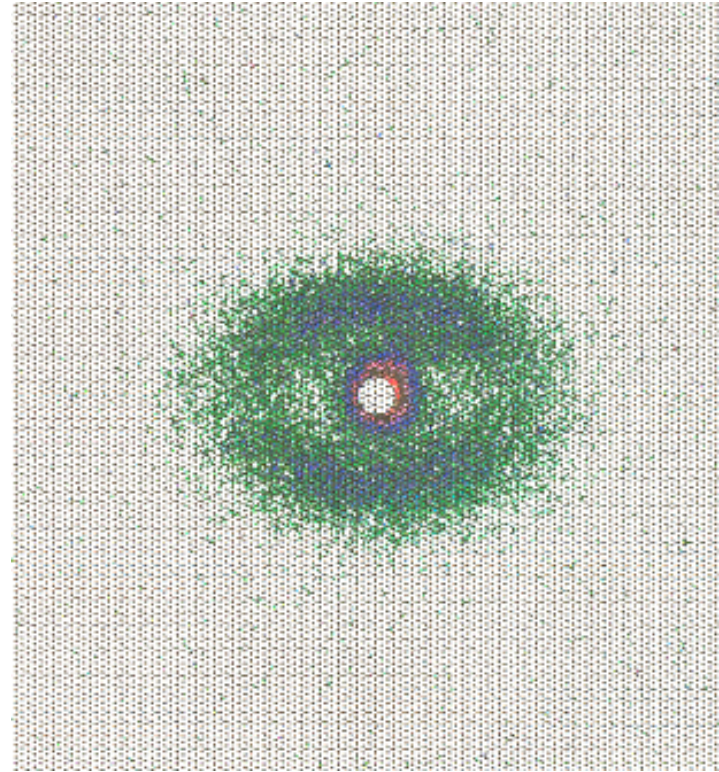
Dispersed Systems as $f(t, \dots)$



Polymers (and Catalysts)



ambient



2X draw

In situ porosity measurements

Quantitative SAXS from
> 2 phase systems

What does it cost
to patent the wrong thing?